# A New Augmented Lagrangian Filter Method

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Thanks to Jonathan Eckstein, Philip Gill, Nick Gould, and Daniel Robinson

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# Active Set Methods for Nonlinear Programming (NLP)

Nonlinear Program (NLP)

$$\underset{x}{\text{minimize}} \ f(x) \quad \text{subject to } c(x) = 0, \ x \geq 0$$

where $f, c$ twice continuously differentiable

**Definition (Active Set)**

Active set: $\mathcal{A}(x) = \{i \mid x_i = 0\}$

Inactive set: $\mathcal{I}(x) = \{1, \ldots, n\} - \mathcal{A}(x)$

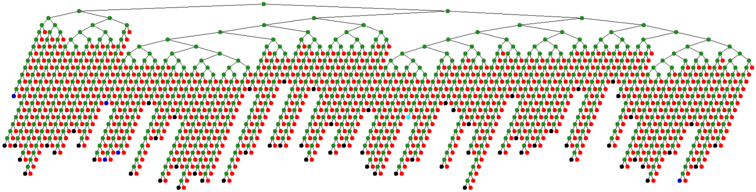
For known optimal active set $\mathcal{A}(x^*)$, just use Newton's method

Goal: develop robust, fast, parallelizable active-set methods

# Active Set Methods for Nonlinear Programming (NLP)

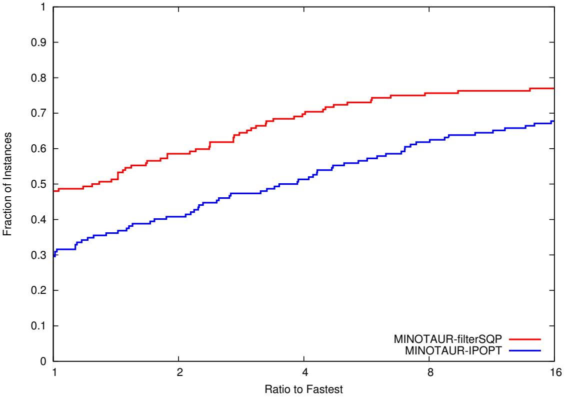
Motivation: mixed-integer nonlinear optimization: $x_i \in \{0, 1\}$

- solve NLP relaxation $x_i \in [0, 1]$
- branch on $\hat{x}_i \notin \{0, 1\}$ ... two new NLPs: $x_i = 0$ or $x_i = 1$
- solve sequence of closely related NLPs



Branch-and-bound solves millions of related NLPs ...

# Active-Set vs. Interior-Point Solvers in MINLP




MINOTAUR with FilterSQP vs IPOPT: CPU time

- FilterSQP warm-starts much faster than IPOPT
- similar results for BONMIN (IBM/CMU) solver

# Outline

# Two-Phase Active-Set Framework for NLP

NLP: $\underset{x}{\text{minimize}}\ f(x)\quad$ subject to $c(x) = 0,\ x \geq 0$

**repeat**

1. Compute cheap first-order step $x^{(k)} + s$, e.g. LP/QP solve
2. Predict active set from $s$: $\mathcal{A}(x^{(k)} + s)$ & $\mathcal{I}(x^{(k)} + s)$
3. Compute second-order *EQP step* on active set:

$$\begin{bmatrix} H_k & A_k \\ A_k^T & \end{bmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \ldots \qquad \text{Newton step}$$

   where $H_k = \nabla^2 L^{(k)}$ and $A_k = \left[\nabla c^{(k)} : I^{(k)}\right]$ active c/s

4. Enforce global convergence & set $k \leftarrow k + 1$

**until** optimal solution found

(Fletcher & de la Maza:89), (Gould & Robinson:10), (Fletcher:11)

Toward scalable nonlinear optimization
$\Rightarrow$ replace LP/QP ... avoid pivoting, i.e. rank-one matrix updates

# Augmented Lagrangian Methods (LANCELOT)

Augmented Lagrangian:

$$L_\rho \quad := \quad f(x) - y^T c(x) + \frac{\rho}{2}\|c(x)\|_2^2$$

With sequences $\omega_k \searrow 0$ and $\eta_k \searrow 0$

**repeat**

1. Find $\omega_k$ optimal solution $\hat{x}^{(k+1)}$ of $\underset{x \geq 0}{\text{minimize}} \; L_\rho(x, y^{(k)})$
2. **if** $\|c(\hat{x}^{(k+1)})\| \leq \eta_k$ **then**

   *update multipliers:* $y^{(k+1)} = y^{(k)} - \rho_k c(\hat{x}^{(k+1)})$

   **else**

   *increase penalty:* $\rho_{k+1} = 2\rho_k$
3. Choose new $(\eta_{k+1}, \omega_{k+1})$; set $k \leftarrow k+1$

**until** (optimal solution found)

see e.g. (Conn, Gould & Toint:95) and (Friedlander, 2002)

# Augmented Lagrangian Methods (LANCELOT)

Advantage of Augmented Lagrangian Methods

- Scalable computational kernels

Disadvantages of Augmented Lagrangian Methods

1. First-order method in multipliers $\Rightarrow$ slow convergence
2. Arbitrary forcing sequences $(\omega_k, \eta_k)$ ... one fits all NLPs?
3. Slow penalty update $\Rightarrow$ slow for infeasible NLPs

Improving augmented Lagrangian methods:

1. Add equality QP step for fast Newton-like convergence
2. Replace forcing sequence $(\omega_k, \eta_k)$ by filter
3. Exploit structure for penalty estimates & use restoration phase

Goal: extend (Friedlander & L., 2008) from QP to NLP

# Outline

# Augmented Lagrangian Filter

Filter $\mathcal{F}$ to replace forcing sequences $(\omega_k, \eta_k)$

**Definition (Augmented Lagrangian Filter)**

- Filter $\mathcal{F}$ is a list of pairs $(\eta(x), \omega(x,y))$ where

$$\omega(x,y) := \| \min\{x, \nabla_x L_0(x,y)\} \| \qquad \ldots \text{ Lagrangian } L_0$$
$$\eta(x) := \|c(x)\| \qquad \ldots \text{ constraint violation}$$

  such that no pair dominates another

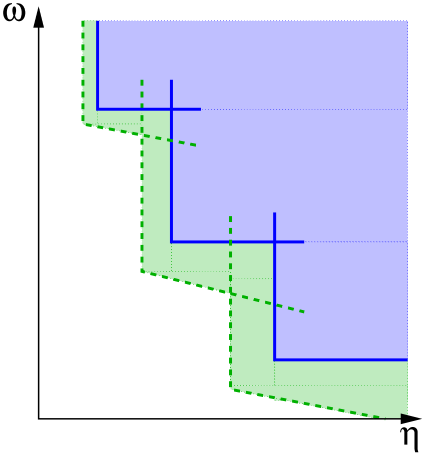
- A point $(x^{(k)}, y^{(k)})$ acceptable to filter $\mathcal{F}$ iff

$$\eta(x^{(k)}) \leq \beta\eta_l \quad \text{or} \quad \omega(x^{(k)}, y^{(k)}) \leq \beta\omega_l - \gamma\eta(x^{(k)}), \quad \forall l \in \mathcal{F}$$

Typically: $\beta = 0.99$, $\gamma = 0.01$

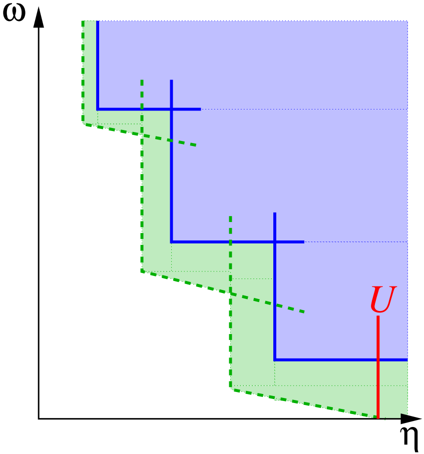
Approximate minimization of $L_\rho(x, y^{(k)})$ until acceptable to filter

# Augmented Lagrangian Filter




- $\omega(x, y) := \| \min\{x, \nabla_x L_0(x, y)\}\|$ and $\eta(x) := \|c(x)\|$

# Augmented Lagrangian Filter




- $\omega(x, y) := \|\min\{x, \nabla_x L_0(x, y)\}\|$ and $\eta(x) := \|c(x)\|$
- Automatic upper bound: $U = \beta/\gamma\omega_{\max}$, because $\omega \geq 0$

# Augmented Lagrangian Filter Method

**while** $(x^{(k)}, y^{(k)})$ *not optimal* **do**

$j = 0$; initialize $\hat{x}^{(j)} = x^{(k)}$, $\hat{\omega}_j = \omega_k$ and $\hat{\eta}_j = \eta_k$

**repeat**

$\hat{x}^{(j+1)} \leftarrow$ approximate $\text{argmin}_{x \geq 0} L_{\rho_k}(x, y^{(k)})$ from $\hat{x}^{(j)}$

**if** *restoration switching condition* **then**

Increase penalty: $\rho_{k+1} = 2\rho_k$ & switch to restoration

... find acceptable $(x^{(k+1)}, y^{(k+1)})$ and set $k = k + 1$

**end**

Provisionally update: $\hat{y}^{(j+1)} = y^{(k)} - \rho_j c(\hat{x}^{(j+1)})$

Compute $(\hat{\eta}_{j+1}, \hat{\omega}_{j+1})$ and set $j = j + 1$

**until** $(\hat{\eta}_j, \hat{\omega}_j)$ *acceptable to* $\mathcal{F}_k$ ;

Set $(x^{(k+1)}, y^{(k+1)}) = (\hat{x}^{(j)}, \hat{y}^{(j)})$

Get $\mathcal{A}^{(k+1)} = \{i : x_i^{(k+1)} = 0\}$ & solve equality QP

**if** $\eta_{k+1} > 0$ **then** add $(\eta_{k+1}, \omega_{k+1})$ to $\mathcal{F}$ ... set $k = k + 1$

**end**

# Approximate Minimization of Augmented Lagrangian

Inner initialization: $j = 0$ and $\hat{x}^{(0)} = x^{(k)}$

For $j = 0, 1, \ldots$ terminate augmented Lagrangian minimization,

$$\hat{x}^{(j+1)} \leftarrow \text{approximate} \ \underset{x \geq 0}{\text{argmin}} \ L_{\rho_k}(x, y^{(k)})$$

when standard sufficient reduction holds:

$$\Delta L_{\rho_k} := L_{\rho_k}(\hat{x}^{(j)}, y^{(k)}) - L_{\rho_k}(\hat{x}^{(j+1)}, y^{(k)}) \geq \sigma \hat{\omega}_j \geq 0$$

E.g. Cauchy step on augmented Lagrangian for fixed $\rho_k$ and $y^{(k)}$

More natural than requiring reduction in F.O. error $\hat{\omega}_j \searrow 0$

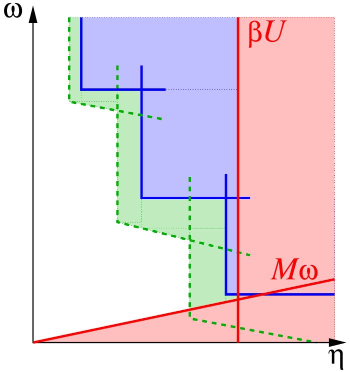
# Switching to Restoration

Goal: Infeasible NLPs $\Rightarrow$ want to find $\underset{x \geq 0}{\text{minimize}} \ \|c(x)\|_2^2$ fast!

Switch to restoration, min $\|c(x)\|$, if

1. $\hat{\eta}_j \geq \beta U$ ... infeasible, or
2. $\hat{\eta}_j \geq M \min(1, \hat{\omega}_j^\tau)$, for $\tau \in [1,2]$ ... infeasible Fritz-John point, or
3. $\| \min(\nabla c^{(j)} c^{(j)}, \hat{x}^{(j)})\| \leq \epsilon$ and $\|c^{(j)}\| \geq \beta \eta_{\min}$ ... infeasible FO Point, where

$$\eta_{\min} := \min_{l \in \mathcal{F}_k} \{\eta_l\} > 0$$




**Lemma (Finite Return From Restoration)**

$\eta_l \geq \eta_{\min} \ \forall l \in \mathcal{F}_k \Rightarrow \exists \ x^{(k+1)}$ *acceptable or restoration converges*

# Second-Order Steps & KKT Solves

- $x^{(k+1)} \leftarrow \underset{x \geq 0}{\text{minimize}}\ L_\rho(x, y^{(k)})$ ... predicts $\mathcal{A}(x^{(k+1)})$
- Accelerate convergence, by solving EQP with $\Delta x_\mathcal{A} = 0$:

$$\begin{bmatrix} \tilde{H}_{k+1} & \tilde{A}_{k+1} \\ \tilde{A}_{k+1}^T & \end{bmatrix} \begin{pmatrix} \Delta x_\mathcal{I} \\ \Delta y \end{pmatrix} = \begin{pmatrix} -\nabla f_\mathcal{I}^{(k+1)} \\ -c(x^{(k+1)}) \end{pmatrix}$$

  where $\tilde{H}_{k+1}$ is "reduced" Hessian wrt bounds ($\Delta x_\mathcal{A} = 0$)
- Line-search: $\alpha_{k+1} \in \{0\} \cup [\alpha_{\min}, 1]$ such that

$$(x^{(k+1)}, y^{(k+1)}) = (\hat{x}^{(k+1)}, \hat{y}^{(k+1)}) + \alpha_{k+1}(\Delta x^{(k+1)}, \Delta y^{(k+1)})$$

  $\mathcal{F}_k$-acceptable
  ... $\alpha_{k+1} = 0$ OK, because $(\hat{x}^{(k+1)}, \hat{y}^{(k+1)})$ was acceptable

# Outline

# Augmented Lagrangian Filter Method

**while** $(x^{(k)}, y^{(k)})$ *not optimal* **do**

$j = 0$; initialize $\hat{x}^{(j)} = x^{(k)}$, $\hat{\omega}_j = \omega_k$ and $\hat{\eta}_j = \eta_k$

**repeat**

$\hat{x}^{(j+1)} \leftarrow$ approximate $\text{argmin}_{x \geq 0} L_{\rho_k}(x, y^{(k)})$ from $\hat{x}^{(j)}$

**if** *restoration switching condition* **then**

Increase penalty: $\rho_{k+1} = 2\rho_k$ & switch to restoration

... find acceptable $(x^{(k+1)}, y^{(k+1)})$ and set $k = k + 1$

**end**

Provisionally update: $\hat{y}^{(j+1)} = y^{(k)} - \rho_j c(\hat{x}^{(j+1)})$

Compute $(\hat{\eta}_{j+1}, \hat{\omega}_{j+1})$ and set $j = j + 1$

**until** $(\hat{\eta}_j, \hat{\omega}_j)$ *acceptable to* $\mathcal{F}_k$ ;

Set $(x^{(k+1)}, y^{(k+1)}) = (\hat{x}^{(j)}, \hat{y}^{(j)})$

Get $\mathcal{A}^{(k+1)} = \{i : x_i^{(k+1)} = 0\}$ & solve equality QP

**if** $\eta_{k+1} > 0$ **then** add $(\eta_{k+1}, \omega_{k+1})$ to $\mathcal{F}$ ... set $k = k + 1$

**end**

# Overview of Convergence Proof

## Assumptions

1. Functions $f(x)$ and $c(x)$ twice continuously differentiable
2. $\|c(x)\| \to \infty$ whenever $\|x\| \to \infty$ ... ignore EQP for analysis

Outline of Convergence Proof

1. Filter $\mathcal{F}_k \Rightarrow$ iterates, $x^{(k)}$ remain in compact set
2. Inner iteration is finite $\Rightarrow \exists$ convergent subsequence
3. Mechanism of filter $\Rightarrow$ limit points are feasible
4. Show limit points are stationary in two cases:
   1. Bounded penalty ... rely on filter
   2. Unbounded penalty ... classical augmented Lagrangian

## Remark

Do not assume compactness, or bounded multipliers!

# Iterates Remain in Compact Set

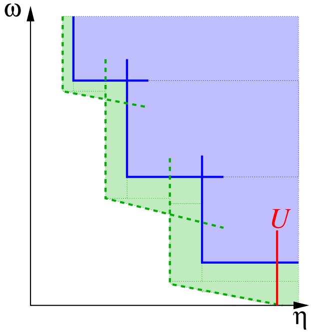
**Lemma (All Iterates Remain in Compact Set)**

*All major and minor iterates, $x^{(k)}$ and $\hat{x}^{(j)}$ are in a compact set, $C$.*

**Proof.**

1. Upper bound on filter $(U = \beta/\gamma\omega_{\max})$
   $\Rightarrow \|c(x^{(k)})\| \leq U$ for all major iterates
2. Switching condition $(\hat{\eta}_j \leq \beta U)$
   $\Rightarrow \|c(\hat{x}^{(j)})\| \leq U$ for all minor iterates
3. Feasibility restoration minimizes $\|c(x)\|$
   $\Rightarrow \|c(x^{(k)})\|$ bounded

$\Rightarrow \|c(^{(k)})\| \leq U$ and $\|c(\hat{x}^{(j)})\| \leq U$




$c(x)$ twice continuously differentiable & $\|c(x)\| \to \infty$ if $\|x\| \to \infty$

$\Rightarrow x^{(k)}, \hat{x}^{(j)} \in C$, compact

# Finiteness of Inner Iteration

## Lemma (Finiteness of Inner Iteration)

*The inner iteration is finite.*

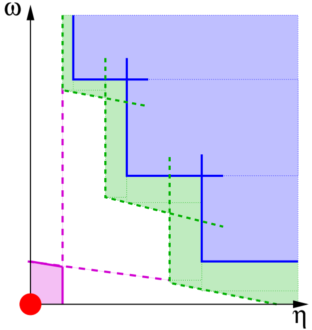
**Proof.** Assume inner iteration not finite $\Rightarrow \exists \hat{x}^* = \lim \hat{x}^{(j)} \in C$

1. Fixed penalty: $\rho_k \equiv \rho < \infty$
2. Sufficient reduction of $L_\rho(x, y^{(k)})$

   $\Rightarrow \Delta L_\rho \geq \sigma \hat{\omega}_j$; assume $\hat{\omega}_j \geq \bar{\omega} > 0$

   $\Rightarrow L_\rho(\hat{x}^{(j)}, y^{(k)})$ unbounded

   ... but $\|c(\hat{x}^{(j)})\|$, $\rho$, and $f(x)$ bounded
3. Contradiction $\Rightarrow \hat{\omega}_j \to 0$, and $\hat{\omega}_* = 0$
4. Switching: $\hat{\eta}_j < M\hat{\omega}_j \Rightarrow \hat{\eta}_* \leq M\hat{\omega}_*$




$\Rightarrow (\hat{\eta}_*, \hat{\omega}_*) = (0, 0)$ and $\exists$ filter acceptable points near $(0, 0)$

# Feasible Limit Points

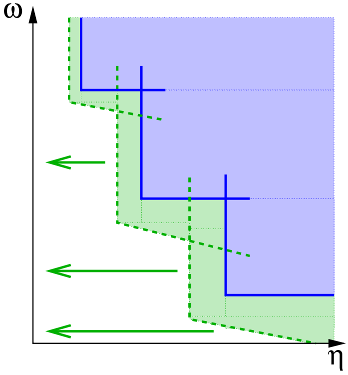
**Lemma (Feasible Limit Points)**

*In outer iteration, feasibility error* $\eta_k = \|c(x^{(k)})\| \to 0$.

**Proof.** Two cases:

1. $\eta_k = 0, \forall k \geq K_0$ ... of course!
2. $\eta_k > 0$, subsequence $\forall k \geq K_0$
   see (Chin & Fletcher, 2003)
   ... envelope $\Rightarrow \eta_k \to 0$

... standard filter argument



# First-Order Optimality

**Lemma (First-Order Stationarity)**

*First-order optimality* $\omega_k = \| \min\{x^{(k)}, \nabla_x L_0^{(k)}\}\| \to 0.$

**Proof.** (1) $\rho_k \le \bar{\rho} < \infty$ and (2) $\rho_k$ unbounded: classical proof

- Assume $\omega_k \ge \bar{\omega} > 0$ & seek contradiction
  $\Rightarrow \Delta L_{\bar{\rho}}^{in} = L_{\bar{\rho}}(x^{(k)}, y^{(k)}) - L_{\bar{\rho}}(x^{(k+1)}, y^{(k)}) \ge \sigma \omega_k \ge \sigma \bar{\omega} > 0$
- First-order multiplier update, $y^{(k+1)} = y^{(k)} - \bar{\rho} c(x^{(k+1)})$

$$\begin{aligned}\Delta L_{\bar{\rho}}^{out} &= L_{\bar{\rho}}(x^{(k)}, y^{(k)}) - L_{\bar{\rho}}(x^{(k+1)}, y^{(k+1)}) \\ &= \Delta L_{\bar{\rho}}^{in} - \bar{\rho} \| c(x^{(k+1)})\|_2^2 \\ &\ge \sigma \bar{\omega} - \rho \| c(x^{(k+1)})\|_2^2\end{aligned}$$

- Feasible limit: $c(x^{(k+1)}) \to 0 \Rightarrow \|c(x^{(k+1)})\|_2^2 \le \sigma \frac{\bar{\omega}}{2\rho}, \; \forall k \ge \bar{K}$
  $\Rightarrow \Delta L_{\bar{\rho}}^{out} \ge \sigma \frac{\bar{\omega}}{2}, \; \forall k \ge \bar{K}$ outer iteration sufficient reduction

# First-Order Optimality (Proof cont.)

- Sufficient reduction at outer iterations: $\Delta L_{\bar\rho}^{out} \geq \sigma \frac{\bar\omega}{2}$
  $\Rightarrow L_{\bar\rho}(x,y) = f(x) - y^T c(x) + \frac{\rho}{2}\|c(x)\|_2^2$ unbounded
- $x^{(k)} \in C$ compact $\Rightarrow f(x)$ and $\|c(x)\|_2^2$ bounded
- Show $y^T c(x) \leq M$ bounded:
  - Feasibility Lemma $\Rightarrow \eta_k = \|c(x^{(k)})\| \to 0$
  - Filter acceptance: Monotone sub-sequences $\eta_k \leq \beta \eta_{k-1}$
  - FO multiplier update: $y^{(k)} = y^{(0)} - \bar\rho \sum_l c^{(l)}$

$$\Rightarrow {y^{(k)}}^T c(x^{(k)}) = \left( y^{(0)} - \bar\rho \sum_l c^{(l)} \right)^T c^{(k)}$$

$$\leq \left(1 + \bar\rho \sum_l \eta_l \right) \eta_k \quad \leq \quad \eta_0 \left( \beta^k + \bar\rho \sum_l \beta^{l+k} \right) \quad \leq \quad M$$

- Contradiction: $L_{\bar\rho}(x,y) = f(x) - y^T c(x) + \frac{\rho}{2}\|c(x)\|_2^2$ bounded
  $\Rightarrow \omega_k \to 0$ ... first-order stationarity

# Outline

# Key Computational Kernels

1. Filter stopping rule readily included in minimization of $L_\rho$
   - $\nabla L_\rho(\hat{x}^{(j+1)}, y^{(k)}) = \nabla L_0(\hat{x}^{(j+1)}, \hat{y}^{(j+1)}) = \hat{\omega}_{j+1}$
2. Approximate minimization of augmented Lagrangian
   - projected gradient plus CG on subspace

$$\left[H_k + \rho A_k A_k^T\right]_{\mathcal{I},\mathcal{I}} \Delta x_{\mathcal{I}} = -\nabla L_\rho(x^{(k)}, y^{(k)})$$

$$\Leftrightarrow \begin{bmatrix} \tilde{H}_k & \tilde{A}_k \\ \tilde{A}_k^T & -\rho^{-1} I \end{bmatrix} \begin{pmatrix} \Delta x_{\mathcal{I}} \\ u \end{pmatrix} = \begin{pmatrix} -\nabla L_\rho(x^{(k)}, y^{(k)}) \\ 0 \end{pmatrix}$$

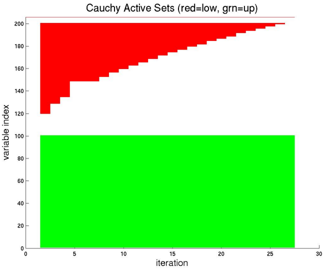
3. KKT system solve
   - $\begin{bmatrix} \tilde{H}_k & \tilde{A}_k \\ \tilde{A}_k^T & \end{bmatrix} \begin{pmatrix} \Delta x_{\mathcal{I}} \\ \Delta y \end{pmatrix} = \ldots$
   - indefinite reduced Hessian $\Rightarrow$ inertia control

$\Rightarrow$ exploit scalable matrix-free solvers based on $H_k, A_k$

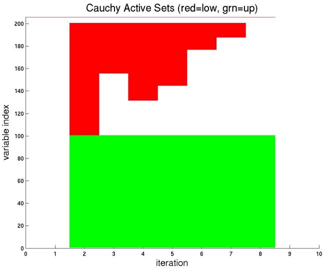
# Active Set Identification for QP `blockqp4_100`

Encouraging preliminary results with QP solver:

Standard AugLag




Filter AugLag




red: lower bound active; green: upper bound active

... filter allows faster changes to $\mathcal{A}$-set

# Conclusions & Open Questions

Augmented Lagrangian Filter:

- augmented Lagrangian to identify optimal active set
- filter replaces forcing sequences in augmented Lagrangian
- second-order step (EQP) for fast convergence
- penalty update based on eigenvalue estimates of KKT matrix

... outline of convergence proof to first-order points

Future Work & Open Questions

- implementation, preconditioners, and numerical experiments
- matrix-free parallel version using TAO & PETSc
- Active-set identification & second-order convergence
- adaptive precision control (Dostal, 2002)
  $\Leftrightarrow$ filter with single entry: $\mathcal{F} = \{(M\|c(x_k)\|, 0)\}$